

# SciCA $\partial$ E 2022



**University of Iceland**  
**July 25 - 29**

**International Conference  
on Scientific Computation and Differential Equations**







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## Foreword

We are very pleased that SciCADE 2022 has met with immense interest despite the troubled times we live in. After more than two years of a pandemic that has changed so much of our world and daily lives, we are happy to finally meet in-person in the beautiful city of Reykjavík. Throughout the many challenges of our present times, we have tried our best to keep the SciCADE community as dynamic, creative and productive as always.

Over 300 international participants are attending SciCADE 2022. The numerous contributions include plenary presentations, mini-symposia, and contributed talks as well as posters. SciCADE 2022 offers a broad diversity of topics within the field of the various applications of scientific computing and differential equations. We are looking very much forward to what will certainly be a fruitful, stimulating meeting.

SciCADE 2022 was made possible due to the hard work of many people, always keen on lending their huge support and precious time. We therefore express our heartfelt thanks to all of those who shared their time and knowledge to make SciCADE 2022 a reality.

We wish you a most enjoyable, productive and rewarding SciCADE 2022.

### Scientific Committee

- Weizhu Bao
- Elena Celledoni
- Sigurdur Hafstein (chair)
- Arieh Iserles
- Alexander Ostermann
- Linda Petzold
- J.M. Sanz-Serna
- Chi-Wang Shu
- Carol Woodward

### Local Organizing Committee

- Sigurdur Hastein (chair)
- Bjorn Birnir
- Peter Giesl
- Hannes Jónsson

### Organizing Support

- Intellegibilis, Lda

## Essential Information

### Venue

The conference will take place at the University of Iceland, in three different buildings: Árnagarður, Askja and Oddi. The campus is in the center of Reykjavík, within walking distance from most hotels. Maps of the campus and all buildings are included on pages 11 to 14.

### Internet Access

Wi-Fi is available throughout the University via the “eduroam” network. If you don’t have access to eduroam, please log into the “CONFERENCE” network.

Should you need any help with connecting, just come by the welcome desk.

### Check-In and Onsite Registration

You can check in (or register onsite, in case you haven’t yet done that online) at the conference welcome desk, situated at the main entrance of the Askja building. The welcome desk will be available during all conference days, from 8:00am until the end of the day at 17:30pm (or until lunch time, in the case of Wednesday and Friday).

### Online Resources

All conference information can be found at the conference website: <https://scicade2021.hi.is/>.

You can also use these direct links:



Conference Website



Conference Program

## Plenary Presentations

### 9am Monday, 25<sup>th</sup> July

**Ari Stern**

Washington University in St. Louis, USA

#### **Structure-preserving hybrid methods**

The classical finite element method uses piecewise-polynomial function spaces satisfying continuity and boundary conditions. Hybrid finite element methods, by contrast, drop these conditions from the function spaces and instead enforce them weakly using Lagrange multipliers. The hybrid approach has several numerical and implementational advantages, which have been studied over the last few decades.

In this talk, we show how this hybrid framework has given new insight into a variety of “structure-preserving” methods for differential equations, including (multi)symplectic methods for Hamiltonian systems, charge-conserving methods for the Maxwell and Yang-Mills equations, and finite element exterior calculus. In particular, this provides a bridge linking “geometric numerical integration” of ODEs to numerical PDEs.

### 4:30pm Monday, 25<sup>th</sup> July

**Dahlquist Prize Talk**

### 9am Tuesday, 26<sup>th</sup> July

**Beth Wingate**

University of Exeter, UK

#### **On the way to the limit: time-parallel algorithms for oscillatory, multiscale PDEs**

Motivated by using exascale computers for high resolution simulations of time-evolution problems, in this talk I will discuss time-parallelism in the context of oscillatory PDEs. I will give an introduction to time-parallel time-stepping methods and then go on to discuss work on understanding and using time-parallel methods for multiscale oscillatory PDEs (fast singular limits) like those found in the atmosphere, ocean, magnetic fields and plasmas. I will give concrete examples from ODEs, such as the swinging spring, and PDEs, such as the rotating shallow water equations. All these problems share the common structure of having a parameter,  $\epsilon$ , associated with purely oscillatory fast frequencies. I will show results of superlinear convergence in the limit as  $\epsilon$  goes to zero, and sketch the proof of convergence for the more important case, when  $\epsilon$  is finite. Time permitting, I will also discuss new directions for this work, including work on multi-level parareal for fast-singular limits and new strategies for using the exponential map with mean-field corrections.

## 4:30pm Tuesday, 26<sup>th</sup> July – New Talent Award

**Yue Feng**

National University of Singapore, Singapore

### **Improved uniform error bounds on time-splitting methods for long-time dynamics of the nonlinear Klein-Gordon equation with weak nonlinearity**

We establish improved uniform error bounds on a second order Strang time-splitting method which is equivalent to an exponential wave integrator for the long-time dynamics of the nonlinear Klein–Gordon equation (NKGE) with weak cubic nonlinearity, whose strength is characterized by  $\varepsilon^2$  with  $0 < \varepsilon \leq 1$  a dimensionless parameter. Actually, when  $0 < \varepsilon \ll 1$ , the NKGE with  $O(\varepsilon^2)$  nonlinearity and  $O(1)$  initial data is equivalent to that with  $O(1)$  nonlinearity and small initial data, the amplitude of which is at  $O(\varepsilon)$ . We begin with a semi-discretization of the NKGE by the second-order time-splitting method and derive a full-discretization by the Fourier spectral method in space. Employing the regularity compensation oscillation (RCO) technique which controls the high frequency modes by the regularity of the exact solution and analyzes the low frequency modes by phase cancellation and energy method, we carry out the improved uniform error bounds at  $O(\varepsilon^2 \tau^2)$  and  $O(h^m + \varepsilon^2 \tau^2)$  for the second-order semi-discretization and full-discretization up to the long time  $T_\varepsilon = T / \varepsilon^2$  with  $T$  fixed, respectively. Extensions to higher order time-splitting methods and the case of an oscillatory complex NKGE are also discussed. Finally, numerical results are provided to confirm the improved error bounds and to demonstrate that they are sharp.

## 9am Wednesday, 27<sup>th</sup> July

**Konstantinos C. Zygalakis**

University of Edinburgh, UK

### **Lyapunov functions, convergence to equilibrium and applications to sampling and optimization**

Optimization and Sampling problems lie in the heart of Bayesian inverse problems. The ability to solve such inverse problems depends crucially on the efficient calculation of quantities relating to the posterior distribution, giving thus rise to computationally challenging high dimensional optimization and sampling problems. In this talk, we will connect the corresponding optimization and sampling problems to the large time behaviour of solutions to (stochastic) differential equations. In addition, using a control theoretical formulation of these equations, we will utilise a set of linear matrix inequalities (applicable in the case of strongly convex potentials) to establish a framework that allow us to deduce their long-time properties as well as deducing the long time properties of their numerical discretisations. In particular, using this framework, we give an alternative explanation for the good properties of Nesterov method for strongly convex functions, as well as highlight the reasons behind the failure of the heavy ball method. Additionally, this framework allows us to study in a unified way the error (in the 2-Wasserstein distance) between the invariant distribution of an ergodic stochastic differential equation and the distribution of its numerical approximation for a number of different integrators proposed in the literature for the overdamped and underdamped Langevin dynamics.



## 9am Thursday, 28<sup>th</sup> July

**J. Nathan Kutz**

University of Washington, USA

### **Dynamical Models from Data**

Machine learning and artificial intelligence algorithms are now being used to automate the discovery of governing physical equations and coordinate systems from measurement data alone. However, positing a universal physical law from data is challenging: (i) An appropriate coordinate system must also be advocated and (ii) simultaneously proposing an accompanying discrepancy model to account for the inevitable mismatch between theory and measurements must be considered. Using a combination of deep learning and sparse regression, specifically the sparse identification of nonlinear dynamics (SINDy) algorithm, we show how a robust mathematical infrastructure can be formulated for simultaneously learning physics models and their coordinate systems. This can be done with limited data and sensors. We demonstrate the methods on a diverse number of examples, showing how data can maximally be exploited for scientific and engineering applications.

## 4:30pm Thursday, 28<sup>th</sup> July

**Caroline Lasser**

Technical University of Munich, Germany

### **Quantum dynamics on the fly**

What do chemical physicists do when simulating the quantum mechanical dynamics of larger molecules? Conventional grid-based discretization becomes unfeasible for molecular systems with more than five to six degrees of freedom, so that tensor and mesh free methods as well as combinations thereof are routinely applied. Our talk will aim at some mathematical grounding of these intriguing computational approaches.

## 9:00am Friday, 29<sup>th</sup> July – Butcher Prize

**John C. Butcher**

University of Auckland, New Zealand

**12:30pm Friday, 29<sup>th</sup> July**

**Gitta Kutyniok**

Ludwig Maximilian University of Munich, Germany

**Scientific Computation meets Artificial Intelligence**

Artificial intelligence is currently leading to one breakthrough after the other, both in public life with, for instance, autonomous driving and speech recognition, and in the sciences in areas such as medical diagnostics or molecular dynamics. A similarly strong impact can currently be witnessed for scientific computation such as for solvers of inverse problems and numerical analysis of partial differential equations. In this lecture, we will first provide an introduction into this new vibrant research area. We will then survey recent advances at the intersection of scientific computation and artificial intelligence, and finally discuss fundamental limitations of such methodologies, in particular, in terms of computability aspects

## Talks and Prizes

### Talks

Each mini-symposium or contributed talk must not last longer than 30 minutes, including time for questions. Chairs will be asked to be very strict about timings.

Sessions will take place in three different buildings: Árnagarður, Askja and Oddi.

All rooms are equipped with full AV facilities and with a Microsoft Windows 10 PC with a PDF reader suitable for beamer presentations, Microsoft Power Point and a media player for basic video playback as well as a web browser. Please bring your presentation on a USB stick and upload it before your session starts. If you intend to present from your own laptop, please ensure that you bring adapters (particularly if you have a Mac). In addition, please bring the files you require for your talk on a USB stick in case there should be any technical issues. Support will be available, if you have problems.

### Prizes

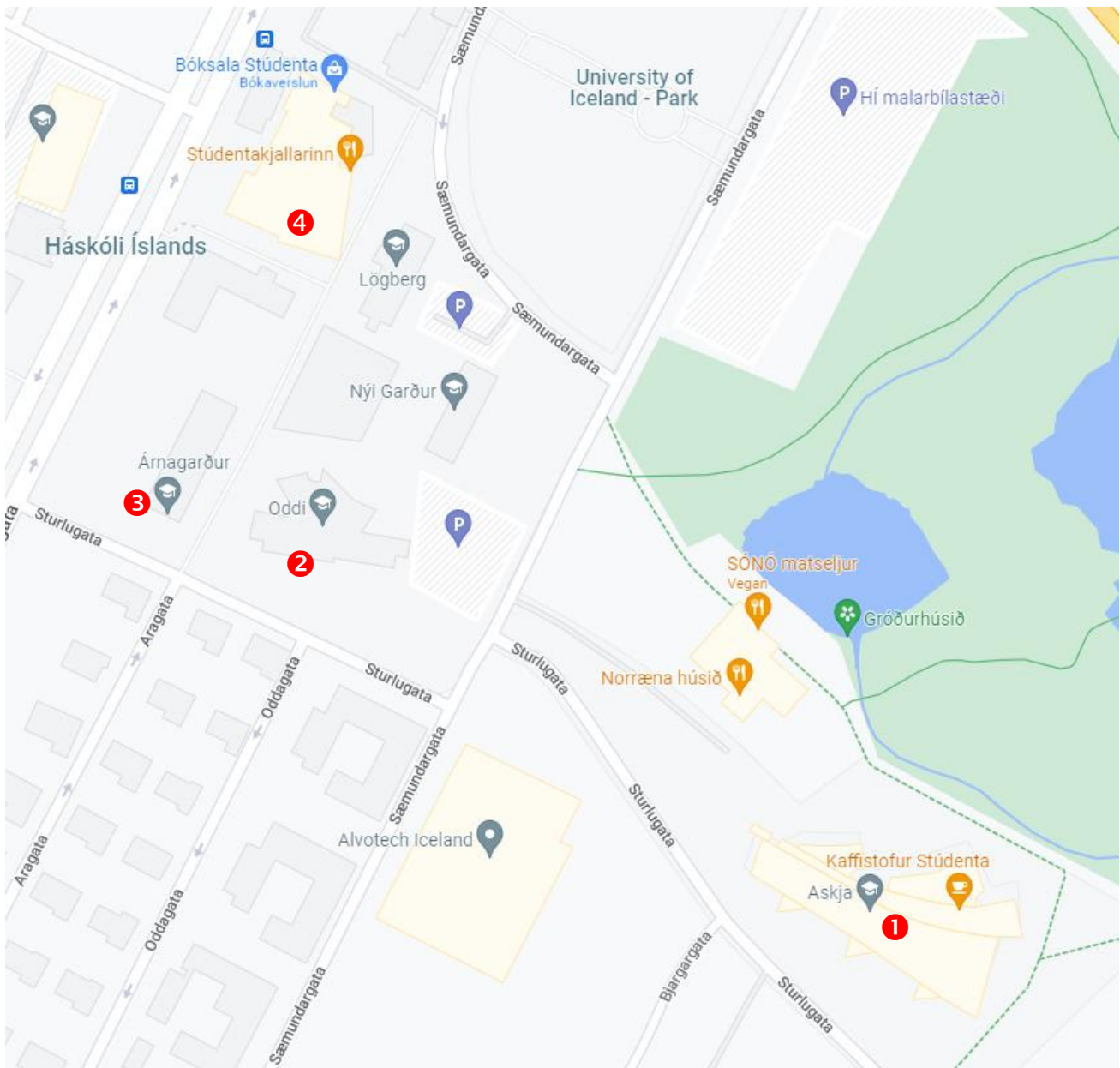
The following prizes will be awarded during SciCADE 2022, at the Askja building:

► **Germund Dahlquist Prize:** This prize, established in 1995, is awarded for original contributions to fields associated with Germund Dahlquist, especially the numerical solution of differential equations and numerical methods for scientific computing. This award will be announced, and a lecture presented by the winner, on Monday at 4:30pm.

► **New Talent Award:** This prize is awarded to the best paper submitted to the panel, on a topic in a field covered by the SciCADE conference. The recipient must be a graduate student or should have obtained a PhD or equivalent degree within the four calendar years prior to the year of the award. This award will be announced, and a lecture presented by the winner, on Tuesday at 4:30pm.

► **Butcher Prize:** This prize, in honour of Prof. John Butcher, is for the best student presentation at SciCADE. It will be awarded on Friday before at 9:00am.

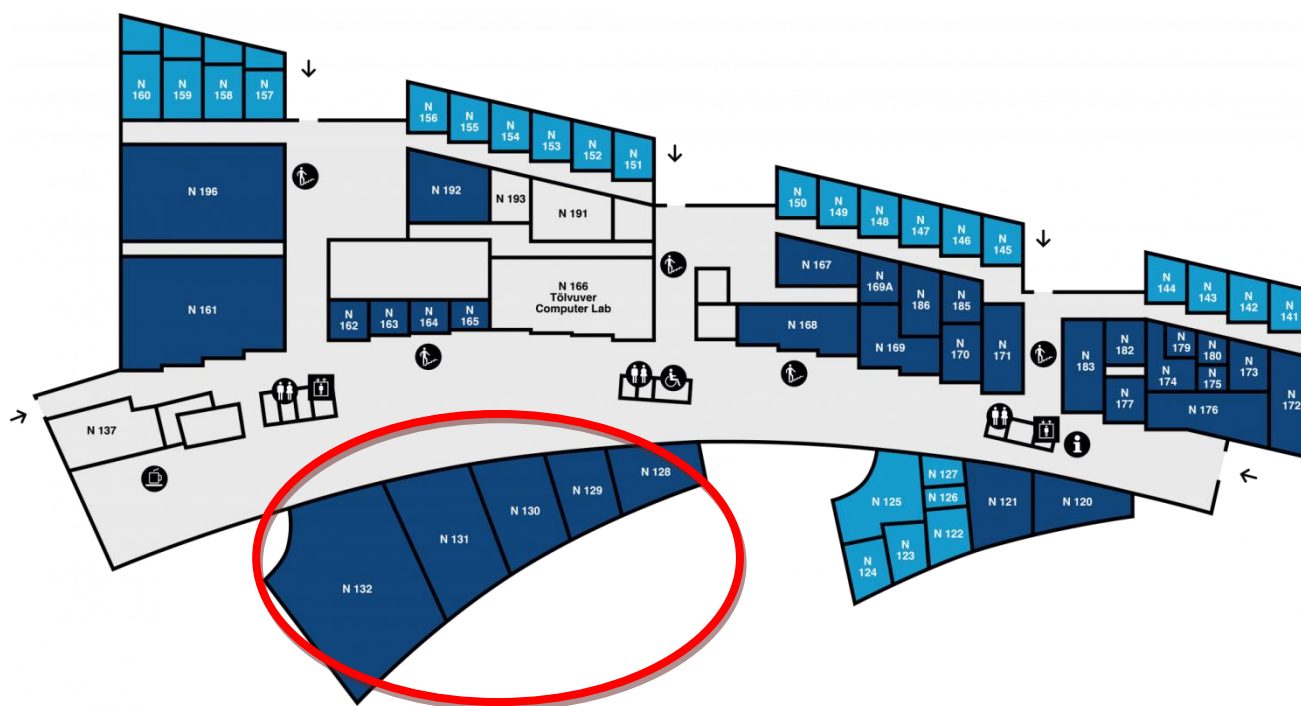
## Campus Maps



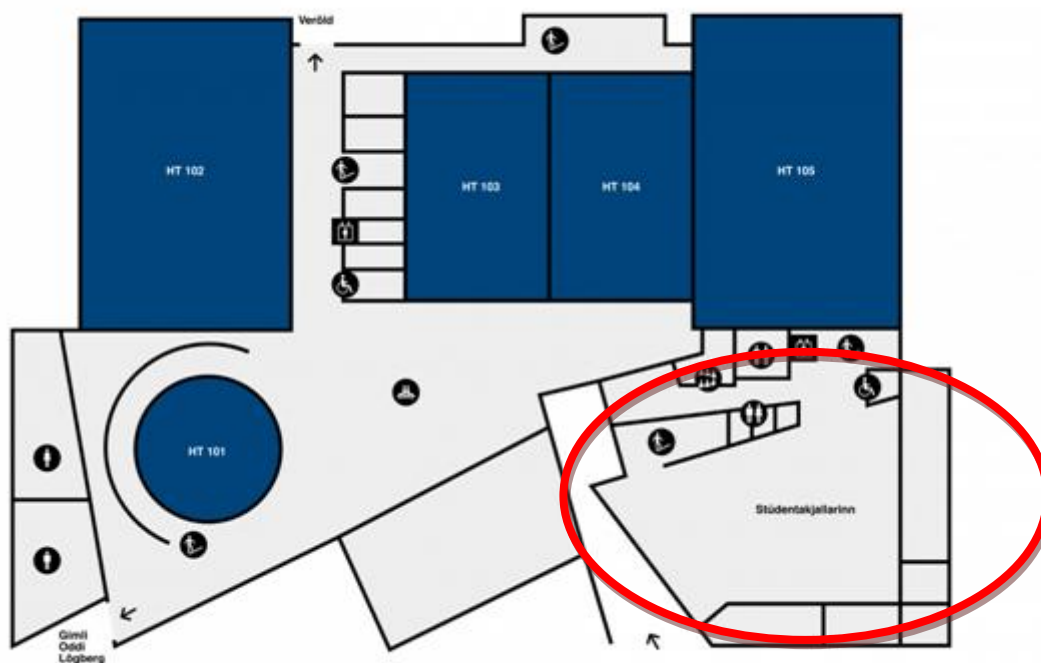
The conference will take place among the following buildings:

- ① **Askja Building:** Welcome desk and “N” rooms.
- ② **Oddi Building:** “O” rooms
- ③ **Árnagarður:** “Á” rooms
- ④ **Háskólatorg:** Coffee-breaks and lunches

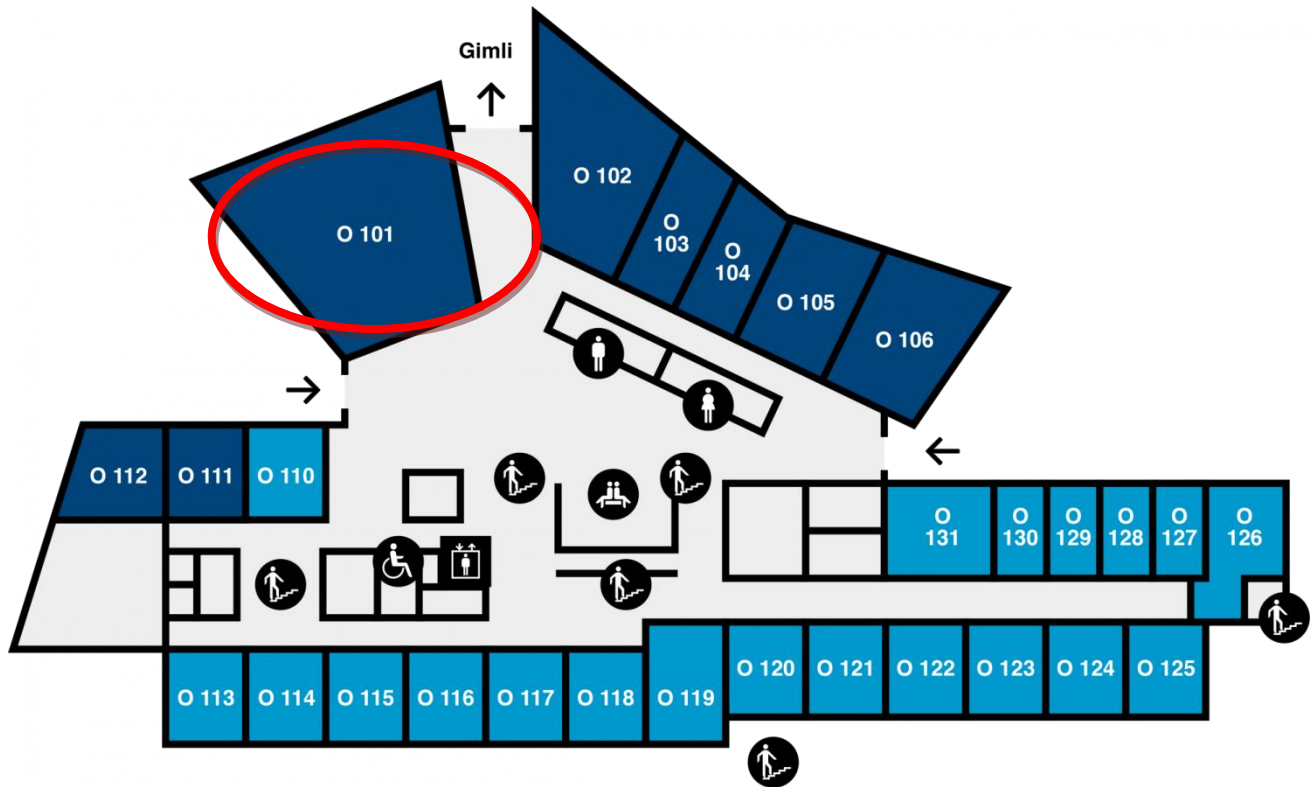
## Askja



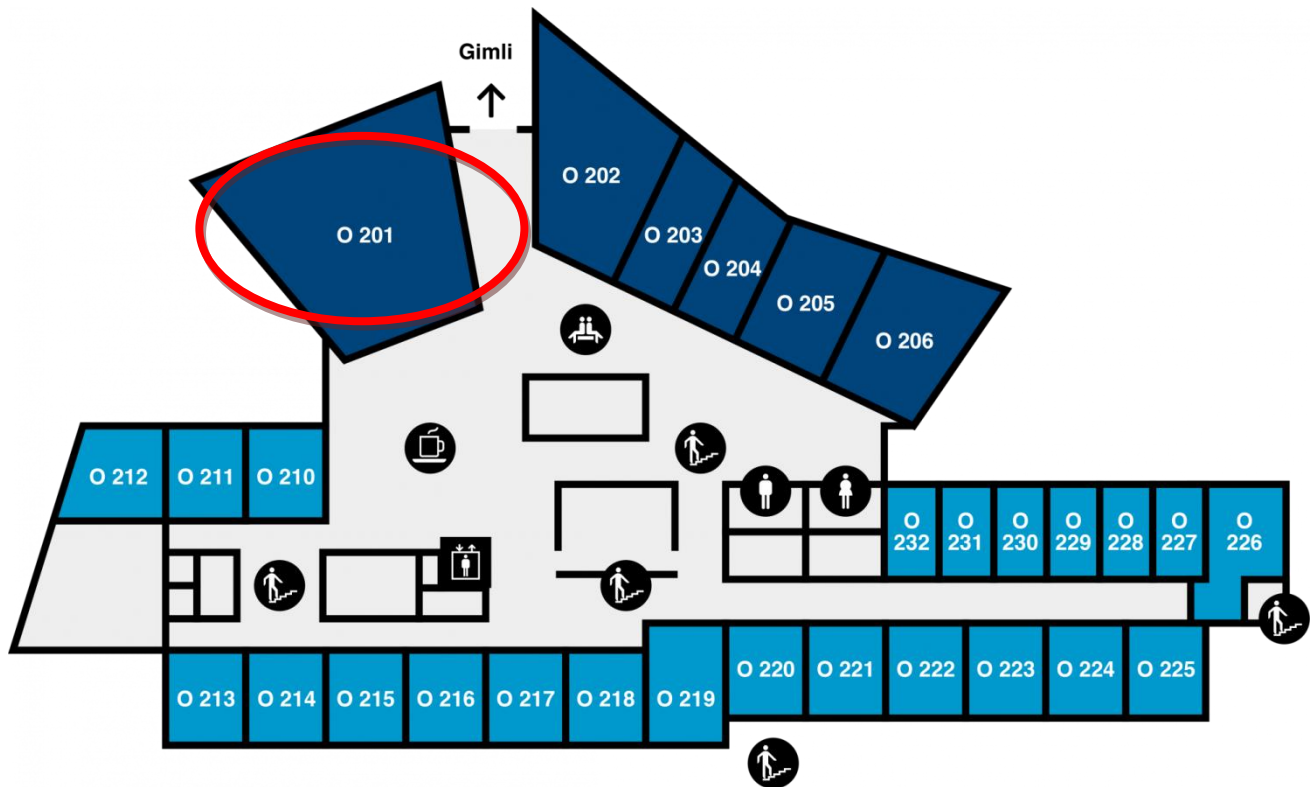
## Háskólatorg



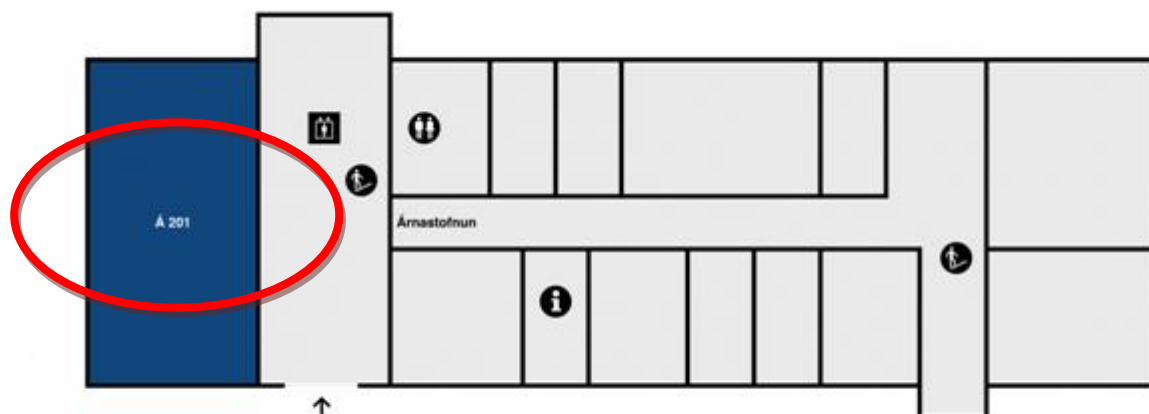
## Oddi - 1<sup>st</sup> Floor



## Oddi - 2<sup>nd</sup> Floor



## Árnagarður – 2<sup>nd</sup> Floor



## Árnagarður – 3<sup>rd</sup> Floor





# Conference Program

	25 July - Monday																		
	N-132	N-131	O-201	O-101	Á-201	Á-301	Á-311	N-130	N-129	N-128									
08:00	Check-in																		
08:30	Opening Session																		
09:00	Plenary Session - Ari Stern																		
09:30	Structure-preserving hybrid methods																		
10:00	Coffee-Break																		
10:30	Contrib Session 1	MS 21 Session 1	Contrib Session 2	MS 17 Session 1	MS 9 Session 1	MS 12 Session 1	MS 10 Session 1	MS 29 Session 1	MS 25 Session 1	MS 4 Session 1									
11:00																			
11:30																			
12:00																			
12:30																			
13:00	Lunch																		
13:30																			
14:00	Contrib Session 3	MS 21 Session 2	Contrib Session 4	MS 17 Session 2	MS 9 Session 2	MS 12 Session 2	MS 10 Session 2	MS 29 Session 2	MS 25 Session 2										
14:30																			
15:00																			
15:30																			
16:00	Coffee-Break																		
16:30	Plenary Session - Dahlquist Prize																		
17:00																			
17:30																			

	26 July - Tuesday																		
	N-132	N-131	O-201	O-101	Á-201	Á-301	Á-311	N-130	N-129	N-128									
08:00	Check-in																		
08:30																			
09:00	Plenary Session - Beth Wingate																		
09:30																			
10:00	Coffee-Break																		
10:30	Contrib Session 5	MS 31 Session 1	MS 34 Session 1	MS 40 Session 1	MS 2 Session 1	MS 5 Session 1	MS 35 Session 1	MS 29 Session 3	MS 23 Session 1	Contrib Session 16									
11:00																			
11:30																			
12:00																			
12:30	Lunch																		
13:00																			
13:30																			
14:00	Contrib Session 6	MS 31 Session 2	MS 34 Session2	MS 40 Session 2	MS 2 Session 2	MS 5 Session 2	MS 35 Session 2	MS 3 Session 1	Contrib Session 7										
14:30																			
15:00																			
15:30																			
16:00	Coffee-Break																		
16:30	Plenary Session - New Talent Award																		
17:00																			
17:30																			



	27 July - Wednesday									
	N-132	N-131	O-201	O-101	Á-201	Á-301	Á-311	N-130	N-129	N-128
08:00	Check-in									
08:30										
09:00	Plenary Session - Konstantinos C. Zygalakis									
09:30										
10:00	Coffee-Break									
10:30	Contrib Session 9	MS 33 Session 1	Contrib Session 8	Contrib Session 10	MS 36 Session 1	MS 13 Session 1	MS 35 Session 3	MS 15 Session 1	MS 11 Session 2	
11:00										
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12:30	Lunch									
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	28 July - Thursday																		
	N-132	N-131	O-201	O-101	Á-201	Á-301	Á-311	N-130	N-129	N-128									
08:00	Check-in																		
08:30																			
09:00	Plenary Session - J. Nathan Kutz																		
09:30																			
10:00	Coffee-Break																		
10:30	MS 19 Session 1	MS 8 Session 1	Contrib Session 11	MS 32 Session 1	MS 6 Session 1	MS 38 Session 1	MS 37 Session 1	MS 16 Session 1	MS 11 Session 1	MS 39 Session 1									
11:00																			
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12:30	Lunch																		
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14:30	MS 19 Session 1	MS 8 Session 2	Contrib Session 12	MS 32 Session 2	MS 6 Session 2	MS 38 Session 2	MS 37 Session 2	MS 16 Session 2		MS 39 Session 2									
15:00																			
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16:00																			
16:30	Coffee-Break																		
17:00	Plenary Session - Caroline Lasser																		
17:30																			

29 July - Friday										
	N-132	N-131	O-201	O-101	Á-201	Á-301	Á-311	N-130	N-129	N-128
08:00	Check-in									
08:30										
09:00	Plenary Session - Butcher Prize									
09:30										
10:00	Coffee-Break									
10:30	MS 37 Session 3	Contrib Session 13						Contrib Session 14	Contrib Session 15	MS 7 Session 1
11:00										
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12:30	Plenary Session - Gitta Kutyniok									
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A better burden may no man bear  
For wanderings wide than wisdom;  
It is better than wealth on unknown ways,  
And in grief a refuge it gives.

Hávamál